Vertical balance equations

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1 Block formulation

Let $\mathbf{x} \in \mathbb{R}^n$ be the "balanced variable" and $\mathbf{v} \in \mathbb{R}^n$ be the "unbalanced variable". They are linked through a "balance operator" $\mathbf{K} \in \mathbb{R}^{n \times n}$:

$$\mathbf{x} = \mathbf{K}\mathbf{v} \tag{1}$$

Let split $\mathbf{x}$ and $\mathbf{v}$ into m blocks, and $\mathbf{K}$ into m^2 square blocks:

$$\begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_m \end{pmatrix} = \begin{pmatrix} \mathbf{K}_{1,1} & \dots & \mathbf{K}_{1,m} \\ \vdots & \ddots & \vdots \\ \mathbf{K}_{m,1} & \dots & \mathbf{K}_{m,m} \end{pmatrix} \begin{pmatrix} \mathbf{v}_1 \\ \vdots \\ \mathbf{v}_m \end{pmatrix} \tag{2}$$

or

$$\mathbf{x}_i = \sum_{j=1}^{m} \mathbf{K}_{i,j} \mathbf{v}_j \tag{3}$$

where the size of each sub-vector $\mathbf{x}_i$ and $\mathbf{v}_i$ is n_i, with $\sum_{i=1}^{m} n_i = n$, and $\mathbf{K}_{i,j} \in \mathbb{R}^{n_i \times n_j}$.

2 Triangular assumption

We assume that the balance operator $\mathbf{K}$ is block-lower-triangular, with identity diagonal blocks:

$$\mathbf{K} = \begin{pmatrix} \mathbf{I}_{n_1} & 0 & \dots & \dots & 0 \\ \mathbf{K}_{2,1} & \mathbf{I}_{n_2} & \ddots & & \vdots \\ \mathbf{K}_{3,1} & \mathbf{K}_{3,2} & \mathbf{I}_{n_3} & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \mathbf{K}_{m,1} & \mathbf{K}_{m,2} & \dots & \mathbf{K}_{m,m-1} & \mathbf{I}_{n_m} \end{pmatrix} \tag{4}$$

Thus, we can simplify equation (3) into:

$$\mathbf{x}_i = \sum_{j=1}^{i-1} \mathbf{K}_{i,j} \mathbf{v}_j + \mathbf{v}_i \tag{5}$$

3 Adjoint

The adjoint of the balance operator is given by:

$$\mathbf{K}^{\mathrm{T}} = \begin{pmatrix} \mathbf{I}_{n_1} & \mathbf{K}_{2,1}^{\mathrm{T}} & \mathbf{K}_{3,1}^{\mathrm{T}} & \dots & \mathbf{K}_{m,1}^{\mathrm{T}} \\ 0 & \mathbf{I}_{n_2} & \mathbf{K}_{3,2}^{\mathrm{T}} & \dots & \mathbf{K}_{m,2}^{\mathrm{T}} \\ \vdots & \ddots & \mathbf{I}_{n} & \ddots & \vdots \\ \vdots & & \ddots & \ddots & \mathbf{K}_{m,m-1}^{\mathrm{T}} \\ 0 & \dots & \dots & 0 & \mathbf{I}_{n_m} \end{pmatrix} \tag{6}$$

so $\mathbf{v} = \mathbf{K}^{\mathrm{T}}\mathbf{x}$ can be expressed as:

$$\mathbf{v}_i = \mathbf{x}_i + \sum_{j=i+1}^{m} \mathbf{K}_{j,i}^{\mathrm{T}} \mathbf{x}_j \tag{7}$$

4 Partial recursive inverse

Equation (5) can be transformed to compute $\mathbf{v}$ knowing $\mathbf{x}$ recursively:

$$\mathbf{v}_i = \mathbf{x}_i - \sum_{j=1}^{i-1} \mathbf{K}_{i,j} \mathbf{v}_j \tag{8}$$

It should be noted that the inverse of $\mathbf{K}_{i,j}$ is not required. This inverse formula is refered to as "partial" since the unbalanced variable $\mathbf{v}$ still appears on the right-hand side.

For the adjoint in equation (7), the same transformation leads to:

$$\mathbf{x}_i = \mathbf{v}_i - \sum_{j=i+1}^{m} \mathbf{K}_{j,i}^{\mathrm{T}} \mathbf{x}_j \tag{9}$$

and must be applied recursively in reverse order (i from m to 1).

5 Full recursive inverse

We assume that for $1 \leq j \leq i$, there are matrices $\mathbf{A}_{i,j} \in \mathbb{R}^{n_i \times n_j}$ such that $\mathbf{v}_i$ can be expressed only as a function of $\mathbf{x}$:

$$\mathbf{v}_i = \sum_{j=1}^{i} \mathbf{A}_{i,j} \mathbf{x}_j \tag{10}$$

Plugging this expression into the partial recursive inverse formula (8), we get:

$$\begin{aligned}
\mathbf{v}_i &= \mathbf{x}_i - \sum_{j=1}^{i-1} \mathbf{K}_{i,j} \mathbf{v}_j \\
&= \mathbf{x}_i - \sum_{j=1}^{i-1} \sum_{k=1}^{j} \mathbf{K}_{i,j} \mathbf{A}_{j,k} \mathbf{x}_k \\
&= \mathbf{x}_i - \sum_{k=1}^{i-1} \sum_{j=k}^{i-1} \mathbf{K}_{i,j} \mathbf{A}_{j,k} \mathbf{x}_k \\
&= \mathbf{x}_i - \sum_{j=1}^{i-1} \sum_{k=j}^{i-1} \mathbf{K}_{i,k} \mathbf{A}_{k,j} \mathbf{x}_j \\
&= \sum_{j=1}^{i-1} \left(- \sum_{k=j}^{i-1} \mathbf{K}_{i,k} \mathbf{A}_{k,j} \right) \mathbf{x}_j + \mathbf{x}_i
\end{aligned} \tag{11}$$

which is consistent with (10) if:

$$\mathbf{A}_{i,j} = -\sum_{k=j}^{i-1} \mathbf{K}_{i,k}\mathbf{A}_{k,j} \text{ (for } j < i) \tag{12a}$$

$$\mathbf{A}_{i,i} = \mathbf{I}_{n_i} \tag{12b}$$

For convenience, we also define the matrices $\mathbf{A}_{i,j}$ for $j > i$ to make the full matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$:

$$\mathbf{A}_{i,j} = \mathbf{A}_{j,i}^{\mathrm{T}} \tag{13}$$

6 Sequential estimation

Since $\mathbf{v}$ is an "unbalanced variable", the component $\mathbf{v}_i$ should be uncorrelated with all the other components:

$$\text{if } j \neq i,\ \operatorname{Cov}\left(\mathbf{v}_i, \mathbf{v}_j\right) = 0 \tag{14}$$

Using the partial recursive inverse (8) for $j < i$, we get:

$$\begin{aligned}
&\operatorname{Cov}\left(\mathbf{v}_i, \mathbf{v}_j\right) = 0 \\
\Leftrightarrow\ &\operatorname{Cov}\left(\mathbf{x}_i - \sum_{k=1}^{i-1} \mathbf{K}_{i,k}\mathbf{v}_k, \mathbf{v}_j\right) = 0 \\
\Leftrightarrow\ &\operatorname{Cov}\left(\mathbf{x}_i, \mathbf{v}_j\right) - \sum_{k=1}^{i-1} \mathbf{K}_{i,k} \operatorname{Cov}\left(\mathbf{v}_k, \mathbf{v}_j\right) = 0
\end{aligned} \tag{15}$$

Using the statistical property (14) of $\mathbf{v}$, the term for which $k = j$ is the only one remaining:

$$\operatorname{Cov}\left(\mathbf{x}_i, \mathbf{v}_j\right) - \mathbf{K}_{i,j} \operatorname{Cov}\left(\mathbf{v}_j, \mathbf{v}_j\right) = 0$$

$$\mathbf{K}_{i,j} = \operatorname{Cov}\left(\mathbf{x}_i, \mathbf{v}_j\right) \operatorname{Cov}\left(\mathbf{v}_j, \mathbf{v}_j\right)^{-1} \tag{16}$$

Using the full recursive inverse (10), we get for $j < i$:

$$\begin{aligned}
\operatorname{Cov}\left(\mathbf{x}_i, \mathbf{v}_j\right) &= \operatorname{Cov}\left(\mathbf{x}_i, \sum_{k=1}^{j} \mathbf{A}_{j,k}\mathbf{x}_k\right) \\
&= \sum_{k=1}^{j} \operatorname{Cov}\left(\mathbf{x}_i, \mathbf{x}_k\right) \mathbf{A}_{j,k}^{\mathrm{T}}
\end{aligned} \tag{17a}$$

$$\begin{aligned}
\operatorname{Cov}\left(\mathbf{v}_j, \mathbf{v}_j\right) &= \operatorname{Cov}\left(\sum_{k=1}^{j} \mathbf{A}_{j,k}\mathbf{x}_k, \sum_{l=1}^{j} \mathbf{A}_{j,l}\mathbf{x}_l\right) \\
&= \sum_{k=1}^{j} \mathbf{A}_{j,k} \sum_{l=1}^{j} \operatorname{Cov}\left(\mathbf{x}_k, \mathbf{x}_l\right) \mathbf{A}_{j,l}^{\mathrm{T}}
\end{aligned} \tag{17b}$$

which allows a computation of the balance operator $\mathbf{K}_{i,j}$ using expression (16).

7 Aggregated formulation

For practical reasons explained later in section 8, we define aggregated quantities:

- the aggregated size $\bar{n}_i = \sum_{j=1}^{i-1} n_j$
- the aggregated vectors $\bar{\mathbf{x}}_i$ and $\bar{\mathbf{v}}_i \in \mathbb{R}^{\bar{n}_i}$:

$$\bar{\mathbf{x}}_i = \begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_{i-1} \end{pmatrix} \quad \text{and} \quad \bar{\mathbf{v}}_i = \begin{pmatrix} \mathbf{v}_1 \\ \vdots \\ \mathbf{v}_{i-1} \end{pmatrix} \tag{18}$$

- the aggregated operator $\overline{\mathbf{K}}_i \in \mathbb{R}^{n_i \times \bar{n}_i}$:

$$\overline{\mathbf{K}}_i = \begin{pmatrix} \mathbf{K}_{i,1} & \dots & \mathbf{K}_{i,i-1} \end{pmatrix} \tag{19}$$

- the aggregated matrix $\overline{\mathbf{A}}_i \in \mathbb{R}^{n_i \times \bar{n}_i}$:

$$\overline{\mathbf{A}}_i = \begin{pmatrix} \mathbf{A}_{i,1} & \dots & \mathbf{A}_{i,i-1} \end{pmatrix} \tag{20}$$

Thus, equation (5) can be rewritten as:

$$\mathbf{x}_i = \overline{\mathbf{K}}_i \bar{\mathbf{v}}_i + \mathbf{v}_i \tag{21}$$

The partial inverse formulation (8) can be rewritten as:

$$\mathbf{v}_i = \mathbf{x}_i - \overline{\mathbf{K}}_i \bar{\mathbf{v}}_i \tag{22}$$

and the full inverse formulation (10) can be rewritten as:

$$\mathbf{v}_i = \overline{\mathbf{A}}_i \bar{\mathbf{x}}_i + \mathbf{x}_i \tag{23}$$

with $\mathbf{A}_{i,j}$ computed as:

$$\mathbf{A}_{i,j} = -\overline{\mathbf{K}}_i \overline{\mathbf{A}}_j^{\mathrm{T}} \tag{24}$$

Finally, we define the matrix $\overline{\overline{\mathbf{A}}}_i \in \mathbb{R}^{\bar{n}_i \times \bar{n}_i}$:

$$\overline{\overline{\mathbf{A}}}_i = \begin{pmatrix} \mathbf{I} & 0 & \dots & 0 \\ \mathbf{A}_{2,1} & \mathbf{I} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ \mathbf{A}_{\mathbf{i-1,1}} & \dots & \mathbf{A}_{\mathbf{i-1,i-2}} & \mathbf{I} \end{pmatrix} \tag{25}$$

to get the aggregated form:

$$\bar{\mathbf{v}}_i = \bar{\bar{\mathbf{A}}}_i \bar{\mathbf{x}}_i \tag{26}$$

The assumption (14) can be rewritten as:

$$\operatorname{Cov}\left(\mathbf{v}_i, \bar{\mathbf{v}}_i\right) = 0 \tag{27}$$

Expanding eqation (27) with the partial recursive inverse (22) we get:

$$\begin{aligned}
&\operatorname{Cov}\left(\mathbf{v}_i, \bar{\mathbf{v}}_i\right) = 0 \\
\Leftrightarrow\ &\operatorname{Cov}\left(\mathbf{x}_i - \bar{\mathbf{K}}_i \bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right) = 0 \\
\Leftrightarrow\ &\operatorname{Cov}\left(\mathbf{x}_i, \bar{\mathbf{v}}_i\right) - \bar{\mathbf{K}}_i \operatorname{Cov}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right) = 0 \\
\Leftrightarrow\ &\bar{\mathbf{K}}_i = \operatorname{Cov}\left(\mathbf{x}_i, \bar{\mathbf{v}}_i\right) \operatorname{Cov}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right)^{-1}
\end{aligned} \tag{28}$$

Using the aggregated full recursive inverse (23) and the aggregated form (26), we get:

$$\begin{aligned}
\operatorname{Cov}\left(\mathbf{x}_i, \bar{\mathbf{v}}_i\right) &= \operatorname{Cov}\left(\mathbf{x}_i, \bar{\bar{\mathbf{A}}}_i \bar{\mathbf{x}}_i\right) \\
&= \operatorname{Cov}\left(\mathbf{x}_i, \bar{\mathbf{x}}_i\right) \bar{\bar{\mathbf{A}}}_i^{\mathrm{T}}
\end{aligned} \tag{29a}$$

$$\begin{aligned}
\operatorname{Cov}\left(\bar{\mathbf{v}}_i, \bar{\mathbf{v}}_i\right) &= \operatorname{Cov}\left(\bar{\bar{\mathbf{A}}}_i \bar{\mathbf{x}}_i, \bar{\bar{\mathbf{A}}}_i \bar{\mathbf{x}}_i\right) \\
&= \bar{\bar{\mathbf{A}}}_i \operatorname{Cov}\left(\bar{\mathbf{x}}_i, \bar{\mathbf{x}}_i\right) \bar{\bar{\mathbf{A}}}_i^{\mathrm{T}}
\end{aligned} \tag{29b}$$

which allows a computation of the balance operator $\bar{\mathbf{K}}_i$ using expression (28).

8 Practical computations

In practice, covariances are sampled from an ensemble. Let $\left\{\widetilde{\mathbf{x}}^1, \ldots, \widetilde{\mathbf{x}}^N\right\}$ be a set of N vectors that samples the distribution of $\mathbf{x}$ and $\left\{\delta\widetilde{\mathbf{x}}^1, \ldots, \delta\widetilde{\mathbf{x}}^N\right\}$ their centered counterparts:

$$\delta\widetilde{\mathbf{x}}^p = \widetilde{\mathbf{x}}^p - \langle\widetilde{\mathbf{x}}\rangle \tag{30}$$

where $\langle\cdot\rangle$ denotes the ensemble mean:

$$\langle\widetilde{\mathbf{x}}\rangle = \frac{1}{N}\sum_{p=1}^{N} \widetilde{\mathbf{x}}^p \tag{31}$$

The covariance $\operatorname{Cov}\left(\mathbf{x}_i, \mathbf{x}_j\right)$ can be estimated from these perturbations by:

$$\widetilde{\operatorname{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right) = \frac{1}{N-1}\sum_{p=1}^{N} \delta\widetilde{\mathbf{x}}_i^p \left(\delta\widetilde{\mathbf{x}}_j^p\right)^{\mathrm{T}} \tag{32}$$

Because of the limited ensemble size N, it can be relevant to filter the covariance matrix with a linear operator $\mathcal{F}$:

$$\overline{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right) = \mathcal{F}\left[\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right)\right] \tag{33}$$

The algorithm to compute the balance operator components using the partial recursive inverse equation (8) is detailed in algorithm 1. Its counterpart using the full recursive inverse equation (10) is detailed in algorithm 2. It should be noted that:

- The first method requires storing the ensemble twice, while the second requires storing more matrices.
- When a filtering $\mathcal{F}$ is applied, both methods can yield different results but there is no theoretical way to know which one is the most accurate.

Algorithm 1 Recursive computation of the balance operator components using the partial recursive inverse formula

Copy the ensemble perturbations:
for $1 \leq p \leq N$ **do**
  $\delta\widetilde{\mathbf{v}}^p = \delta\widetilde{\mathbf{x}}^p$
end for

for $1 \leq i \leq m$ **do**
  for $1 \leq j < i$ **do**
    Estimate the cross-covariance between $\mathbf{x}_i$ and $\mathbf{v}_j$:
$$\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right) = \frac{1}{N-1}\sum_{p=1}^{N} \delta\widetilde{\mathbf{x}}_i^p \left(\delta\widetilde{\mathbf{v}}_j^p\right)^{\mathrm{T}}$$
    Filter the cross-covariance between $\mathbf{x}_i$ and $\mathbf{v}_j$:
$$\overline{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right) = \mathcal{F}\left[\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right)\right]$$
    Inverse $\overline{\mathrm{Cov}}\left(\mathbf{v}_j, \mathbf{v}_j\right)$ to get $\overline{\mathrm{Cov}}\left(\mathbf{v}_j, \mathbf{v}_j\right)^{-1}$
    Compute the balance operator component $\mathbf{K}_{i,j}$:
$$\mathbf{K}_{i,j} = \overline{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right)\overline{\mathrm{Cov}}\left(\mathbf{v}_j, \mathbf{v}_j\right)^{-1}$$

    Update the unbalanced ensemble perturbations:
    for $1 \leq p \leq N$ **do**
      $\delta\widetilde{\mathbf{v}}_i^p \leftarrow \delta\widetilde{\mathbf{v}}_i^p - \mathbf{K}_{i,j}\delta\widetilde{\mathbf{v}}_j^p$
    end for
  end for

  if $i < m$ **then**
    Estimate the auto-covariance of $\mathbf{v}_i$:
$$\widetilde{\mathrm{Cov}}\left(\mathbf{v}_i, \mathbf{v}_i\right) = \frac{1}{N-1}\sum_{p=1}^{N} \delta\widetilde{\mathbf{v}}_i^p \left(\delta\widetilde{\mathbf{v}}_i^p\right)^{\mathrm{T}}$$
    Filter the auto-covariance of $\mathbf{v}_i$:
$$\overline{\mathrm{Cov}}\left(\mathbf{v}_i, \mathbf{v}_i\right) = \mathcal{F}\left[\widetilde{\mathrm{Cov}}\left(\mathbf{v}_i, \mathbf{v}_i\right)\right]$$
  end if
end for

Algorithm 2 Recursive computation of the balance operator components using the full recursive inverse formula

for $1 \leq i \leq m$ **do**
  for $1 \leq j \leq i$ **do**
    Estimate the cross-covariance between $\mathbf{x}_i$ and $\mathbf{x}_j$:
$$\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right) = \frac{1}{N-1}\sum_{p=1}^{N} \delta\widetilde{\mathbf{x}}_i^p \left(\delta\widetilde{\mathbf{x}}_j^p\right)^{\mathrm{T}}$$
    Filter the cross-covariance between $\mathbf{x}_i$ and $\mathbf{x}_j$:
$$\overline{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right) = \mathcal{F}\left[\widetilde{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right)\right]$$
  end for
end for

for $1 \leq i \leq m$ **do**
  for $1 \leq j < i$ **do**
    Compute the cross-covariance between $\mathbf{x}_i$ and $\mathbf{v}_j$:
$$\overline{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right) = \sum_{k=1}^{j-1} \overline{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_k\right)\mathbf{A}_{j,k}^{\mathrm{T}} + \overline{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{x}_j\right)$$
    Inverse $\overline{\mathrm{Cov}}\left(\mathbf{v}_j, \mathbf{v}_j\right)$ to get $\overline{\mathrm{Cov}}\left(\mathbf{v}_j, \mathbf{v}_j\right)^{-1}$
    Compute the balance operator component $\mathbf{K}_{i,j}$:
$$\mathbf{K}_{i,j} = \overline{\mathrm{Cov}}\left(\mathbf{x}_i, \mathbf{v}_j\right)\overline{\mathrm{Cov}}\left(\mathbf{v}_j, \mathbf{v}_j\right)^{-1}$$
  end for

  for $1 \leq j < i$ **do**
    Compute the matrix $\mathbf{A}_{i,j}$:
$$\mathbf{A}_{i,j} = -\sum_{k=j}^{i-1} \mathbf{K}_{i,k}\overline{\mathbf{A}}_{k,j}$$
  end for

  if $i < m$ **then**
    Compute temporary matrices $\mathbf{S}_{k,i}$:
    for $1 \leq k \leq i$ **do**
$$\mathbf{S}_{k,i} = \sum_{l=1}^{k} \overline{\mathrm{Cov}}\left(\mathbf{x}_k, \mathbf{x}_l\right)\mathbf{A}_{i,l}^{\mathrm{T}} + \sum_{l=k+1}^{i-1} \overline{\mathrm{Cov}}\left(\mathbf{x}_l, \mathbf{x}_k\right)^{\mathrm{T}}\mathbf{A}_{i,l}^{\mathrm{T}} + \overline{\mathrm{Cov}}\left(\mathbf{x}_k, \mathbf{x}_i\right)$$
    end for

    Compute the auto-covariance of $\mathbf{v}_i$:
$$\overline{\mathrm{Cov}}\left(\mathbf{v}_i, \mathbf{v}_i\right) = \sum_{k=1}^{i-1} \mathbf{A}_{i,k}\mathbf{S}_{k,i} + \mathbf{S}_{i,i}$$
  end if
end for